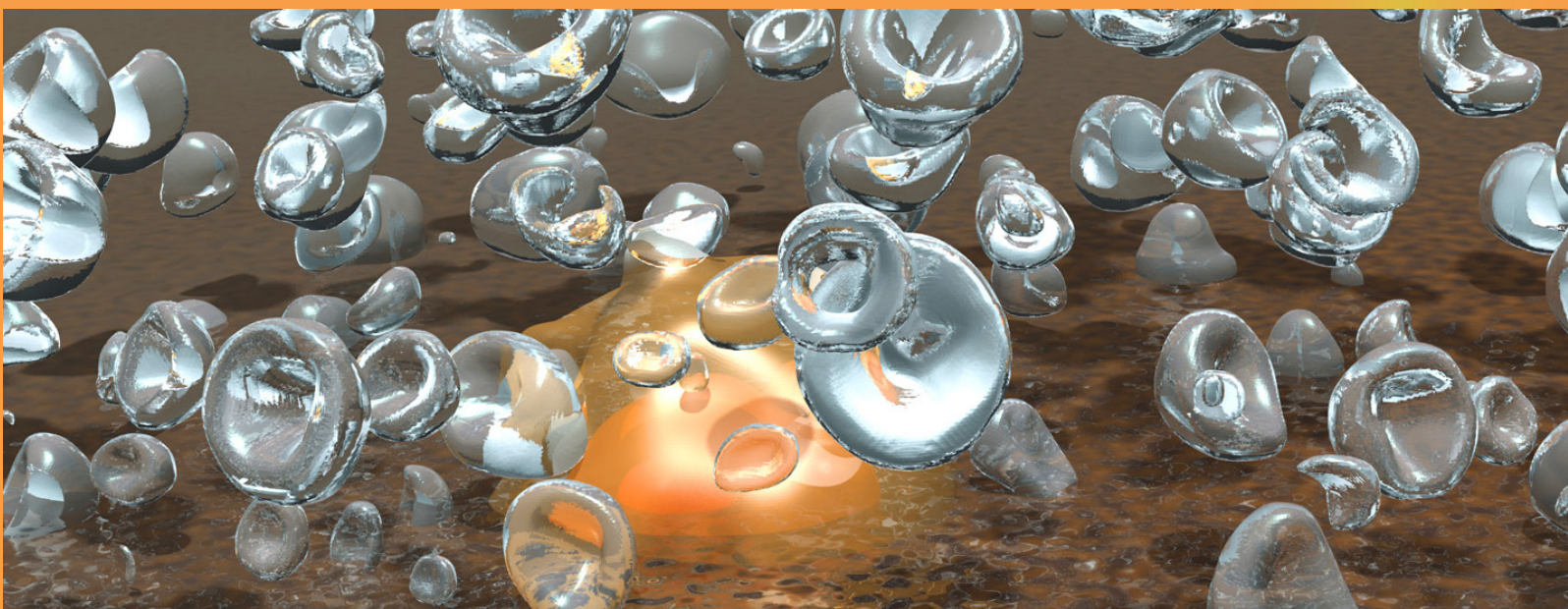


# Science and Technology UPDATE

November/December 2013



SCIENCE ON A MISSION



LLNL-MI-648539

### GORDON BELL PRIZE FOR SEQUOIA SIMULATION OF “VIOLENT BUBBLES”

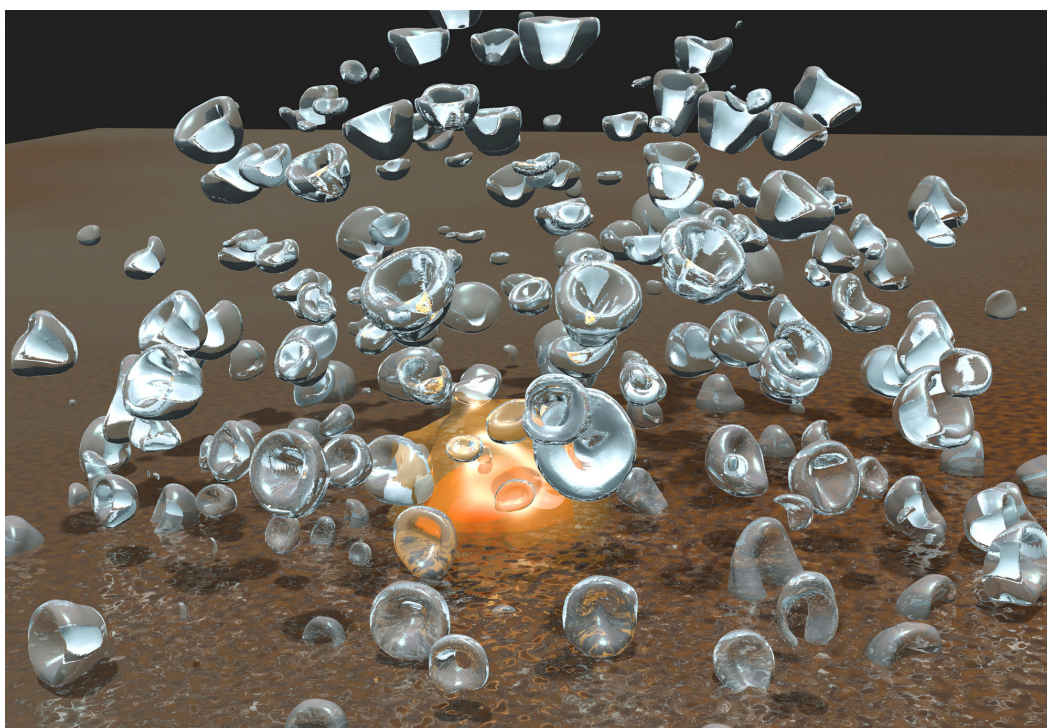
A record-setting simulation run on the Sequoia supercomputer was awarded the Gordon Bell Prize in the peak performance category. Using a record number of 6.4 million threads on Livermore’s IBM BlueGene/Q machine, the fluid dynamics **simulation of cloud cavitation collapse** employed 13 trillion cells—making it the largest simulation ever in fluid dynamics—and achieved a computational speed of 14.4 petaflops (73% of Sequoia’s theoretical peak). The **simulation** was conducted by researchers from

the power of the phenomenon to destroy cancer cells or deliver drugs more effectively in the human body. (Image courtesy ETH Zurich.)

### LAB CONTRIBUTES TO NOBEL PEACE PRIZE WINNER

The Laboratory’s **Forensic Science Center** is one of only two U.S. laboratories that is accredited to conduct chemical weapons-related testing for the Organization for the Prohibition of Chemical Weapons (OPCW), which **received the 2013 Nobel Peace Prize** “for its extensive efforts

to eliminate chemical weapons.” The testing that the Laboratory performs is to detect, in samples, not only traces of the dangerous chemicals themselves but also their precursors—other chemicals used to make chemical weapons. Said Forensic Science Center head Brad Hart, “Our OPCW work, along with the efforts of the other 20 laboratories, provides an important international security capability by helping to verify and ensure compliance with the Chemical Weapons Convention.” The conven-



LLNL, ETH Zurich, IBM Research, and the Technical University of Munich and resolved unique phenomena associated with “cloud cavitation collapse”—clouds of collapsing bubbles. The vastly improved performance of the new simulation paves the way for research on a wide range of applications, such as avoiding damage from cavitation collapse to turbine components and propellers and harnessing

tion, which came into force in 1997 and bans the production, stockpiling, and use of such weapons, is implemented through the OPCW. To maintain its OPCW accreditation, Lawrence Livermore, like any other scientific laboratory, must undergo challenging tests of chemical sample analysis proficiency and maintain a three-year rolling average of at least two “A” grades and one “B.”

#### About the Cover

A record-setting simulation of an energetic cloud of collapsing bubbles performed on the Sequoia supercomputer at LLNL won the Gordon Bell Prize in 2013. See article on this page.



## LABORATORY WINS FOUR TECH TRANSFER AWARDS

Lawrence Livermore garnered four awards in the Far West Regional competition in the latest Federal Laboratory Consortium **awards for excellence in technology transfer**. DNA-Tagged Reagents for Aerosol Experiments (**DNATrax**), a safe material that can be used to reliably and rapidly diagnose airflow patterns and problems as part of vulnerability assessments, for instance, won an Outstanding Technology Development Award. Two Outstanding Partnership Awards were won—one for **Rapid Viability Polymerase Chain Reaction**, a fast method for detecting viable anthrax-causing spores and developed in collaboration with the Environmental Protection Agency; and another for the **Earth System Grid Federation**, which the Lab developed with 11 partner institutions to support the **Coupled Model Intercomparison Project**. Finally, an Outstanding Commercialization Success Award was presented to the Laboratory and Pleasanton, CA-based startup QuantaLife (and its successor company) for commercializing an LLNL digital polymerase chain reaction (PCR) technology as the line of **Droplet Digital™ PCR** systems, known as the most accurate genetic analysis platform currently available. These four awards—which bring to 22 the number of Far West Regional awards the Laboratory has won since 2007—**were presented to LLNL staff** in December.

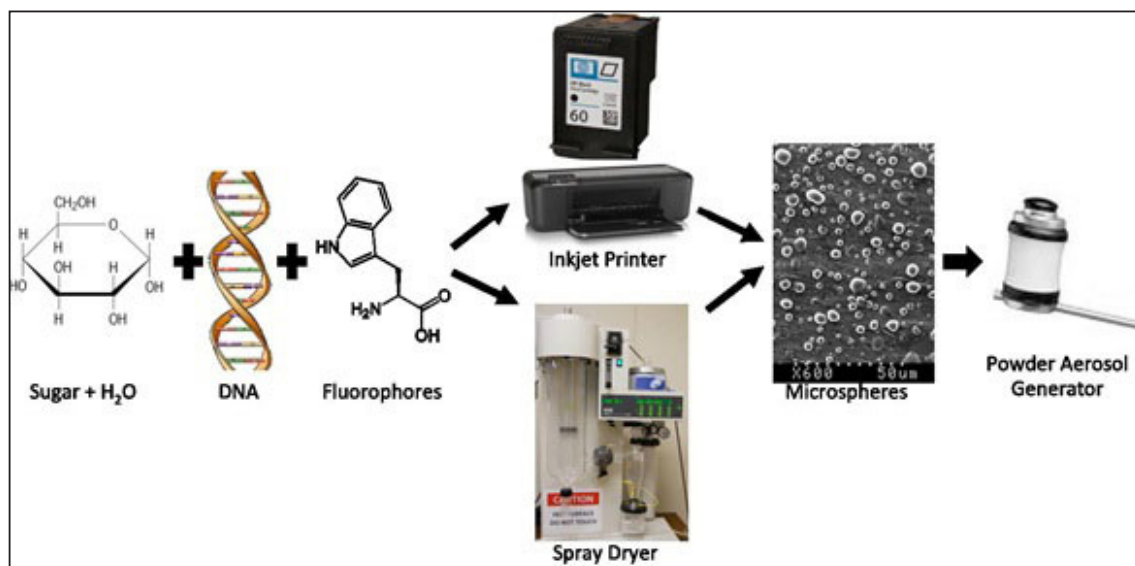
The image illustrates the process by which DNATrax is used to create particles “barcoded” with DNA and, from them, generate an aerosol, using even an ordinary inkjet printer.

## SECOND AWARD FOR PHYSICIST FOR DTRA NUCLEAR FORENSICS

Lab physicist Roger White has received a second award from the Defense Threat Reduction Agency (DTRA) for his work in post-detonation nuclear forensics. In the latest nod, Roger was named “top contributor” of the third quarter of fiscal 2013 for leading a 55-person, multiple-organization “red team” that successfully developed and executed a simulated terrorist nuclear event occurring in the United States. The exercise was part of a program to develop an enhanced capability to forensically reconstruct such an attack rapidly and accurately using data from ground-based diagnostics. In addition to Roger, the Livermore team also includes radiochem-



ist Yves Dardenne, physicists Britton Chang and Mark May, computer scientist Steve Anderson, engineer Craig Halvorson, seismologist Artie Rodgers, and technical nuclear forensics program manager Alan Ross.



### SUCCESSFUL END OF 20-YEAR U.S.-RUSSIA EFFORT TO RECOVER URANIUM

On November 14, U.S. Energy Secretary Moniz **announced the final shipment** of low-enriched uranium (LEU) derived from Russian weapons-origin highly enriched uranium (HEU) under the 1993 U.S.-Russia HEU Purchase Agreement. Designed to prevent weapons-grade uranium from dismantled Russian nuclear weapons from falling into the hands of terrorists or rogue states, the agreement was a key implementation of the Treaty on the Nonproliferation of Nuclear Weapons. Under the agreement, Russia down-blended 500 metric tons of HEU, equivalent to 20,000 nuclear warheads, into LEU, thus achieving the agreement's original target for the 20-year period. The resulting LEU has been delivered to the United States, fabricated into nuclear fuel, and used in nuclear power plants to generate nearly ten percent of all U.S. electricity over the past 15 years.

Lawrence Livermore, as lead laboratory for the program, supplied personnel for the monitoring trips, provided all of the health physics support, maintained

a repository of the collected monitoring data (available to both sides in the interest of transparency), and developed and deployed radiation detection equipment, such as a portable nondestructive assay system used to verify the contents of uranium containers (photo) without breaking their seals. (Image courtesy of USEC.)

### RECOVERING POTENTIAL “DIRTY BOMB” MATERIAL FROM RUSSIAN ARCTIC

NNSA recently announced **the successful removal** of 14 Russian radioisotope thermoelectric generators (RTGs) from an Arctic zone known as the Northern Sea Route in partnership with the Russian Federation. The RTGs, which contain high-activity radioactive sources, were used for many years in Russia to generate electrical power at remote locations, and their removal by Russian technical specialists involved work in challenging locations north of the Arctic Circle. The RTGs were transported by helicopter, ship, and truck to a secure facility, where they

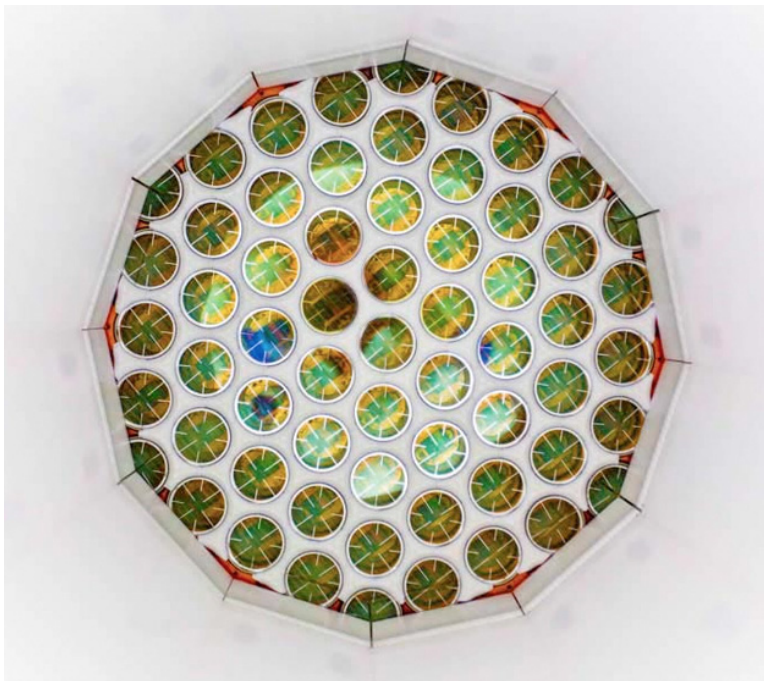
will be disassembled and the radioactive heat sources sent to secure long-term storage. Livermore's Bill Abramson and Steve Porter supported this recovery project for NNSA's Global Threat Reduction Initiative, which LLNL has been working with for the last decade to recover a total of 482 RTGs throughout Russia and secure more than 20 million curies of vulnerable radioactive material. This latest removal marks the completion of NNSA's RTG recovery along the Northern Sea Route.





### LUX PROVES ITSELF WORLD'S MOST SENSITIVE DARK-MATTER DETECTOR

Scientists at the Large Underground Xenon (LUX) Experiment—including three from LLNL—announced that data recently obtained show that LUX is the most sensitive dark matter detector in the world. **Lowered into position** last year a mile underground at the Sanford Underground Research Facility, in Lead, South Dakota, the LUX detector was built to detect weakly interacting massive particles (WIMPs)—the leading theoretical candidates for dark matter—and exhibited a peak sensitivity at a WIMP mass of 33 GeV/c<sup>2</sup>, with a sensitivity more than 20 times better than previous experiments for low-mass WIMPs. Although LUX has not yet detected any dark matter candidates, “coming up empty-handed is a vital part of science,” **as *The Economist* pointed out**. For instance, if the results of the earlier **Cryogenic Dark Matter Search** were accurate, LUX should have seen approximately 1,500 WIMPs in 3 months. Livermore’s work on LUX began as a natural extension of its work in detectors for nonproliferation applications. Groundbreaking work at LLNL that set the stage for LUX was supported by the LDRD Program, including a strategic initiative **(10-SI-015)** led by Adam Bernstein, one of the three Livermore scientists closely involved in LUX. Said Adam, “LUX is a great example of the powerful benefit of LLNL’s internal science funding [LDRD] for fundamental science.” The photo shows the LUX photomultiplier tube mounting structure, which was designed and built at LLNL.



### ARTIFICIAL RETINA MAKES “INVENTION OF THE YEAR” LISTS

*Time* magazine has named the Argus II retinal prosthesis—widely referred to as a “bionic eye”—as **one of the 25 best inventions of 2013**. The Argus II, which is marketed by Second Sight Medical Products, Inc., was also named by *Popular Science* as **the top innovation of the year**. Earlier this year, the technology became the first-ever retinal prosthesis **approved in the U.S. by the FDA** for blind persons with end-stage retinitis pigmentosa. The Argus II is the culmination of a **multi-institutional DOE project** whose efforts at Livermore, Sandia, and Los Alamos National Laboratories received crucial early-stage **support by the LDRD Program**. The Argus II package includes an eyeglass-mounted video camera (in the center of the eyeglasses) that sends video signals to a microprocessor for conversion to electronic signals, which are transmitted wirelessly from outside the body to the heart of the technology—an electrode array implanted in the back of the eye. The implant stimulates the retina’s remaining cells, which transmit the visual information along the optic nerve to the brain, creating the perception of light patterns.

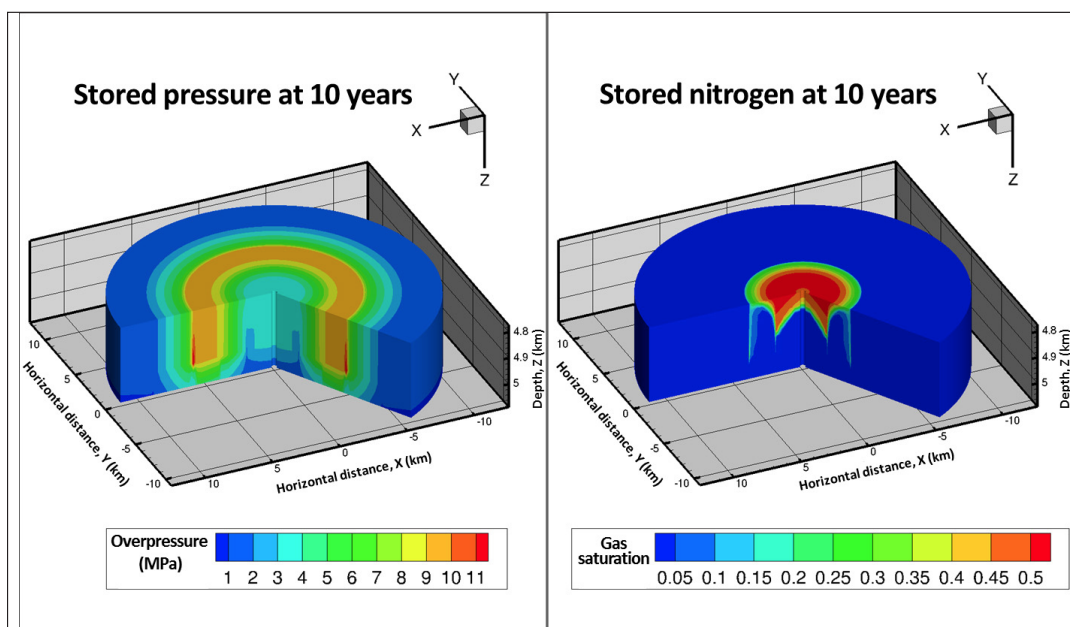
## SIX APS FELLOWS ELECTED

Four scientists were recently named fellows of the American Physical Society (APS), bringing the 2013 total to six. Charles Cerjan was recommended by the APS Division of Atom, Molecular, and Optical Physics for “seminal contributions to time-dependent Schrodinger equation propagation algorithms and their applications, the development of laser-produced plasma sources for advanced lithography, and the investigation of the basic mechanism of magnetic multilayer material response and its application to magnetic storage devices.” Marilyn Schneider was recommended by the APS Topical Group on Instrumentation and Measurement Science for her “outstanding contributions to x-ray measurements from laser-produced plasmas.” Eric Schwegler was recommended by the APS Division of Computational Physics for his “important contributions to the development of linear scaling electronic structure theory and the use of first-principles methods to examine the properties of aqueous solutions, nanomaterials, and matter under extreme conditions.” Ian Thompson was recommended by the APS Division of Nuclear Physics for his “development and application of all-order treatments of nuclear-cluster dynamics in peripheral reactions, leading to a new understanding of halo nuclei within a few-body framework.”

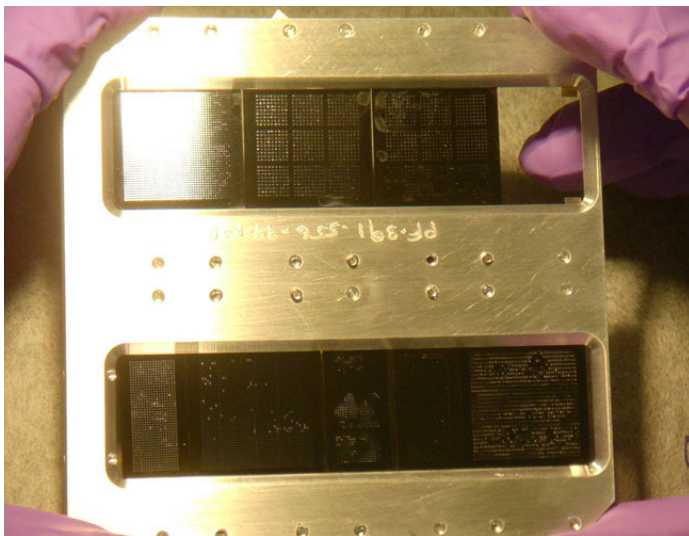
## ANNOUNCED AT AGU CONFERENCE: BETTER WAY TO HARVEST GEO HEAT AND STORE CO<sub>2</sub>

At the **2013 fall meeting** of the American Geophysical Union, LLNL researchers debuted a new design for a geothermal power plant that not only harvests heat more effectively than the conventional approach but does so with sequestered carbon dioxide, thereby reducing climate-impacting emissions in two ways. The team of earth scientists, led by Tom Buscheck, explained that by adding liquid carbon dioxide and even some nitrogen to the water currently used in the concentric configuration of wells, the resultant mixture will more effectively transfer heat from an underground geothermal source to the surface, where it can be used to generate steam and drive turbines, for instance. Adding nitrogen to the mix would further improve the wells’ ability to store large amounts of heat for long periods, giving plant operators the flexibility to synchronize energy production with demand patterns. Together, these improvements—**described in a paper in *Greenhouse Gases Science and Technology***—would make the concentric-well approach viable even for smaller hot spots, further increasing the amount of energy producible in the nation from geothermal sources. The geothermal plant envisioned by Tom and team could also be paired with a

coal-fired power plant, utilizing carbon dioxide captured via scrubbing from the plant’s emissions. The figures show the size and shape of the concentric wells that would be created over a geothermal source; the predicted pressure, which would still be sufficient for energy generation; and nitrogen content after 10 years.



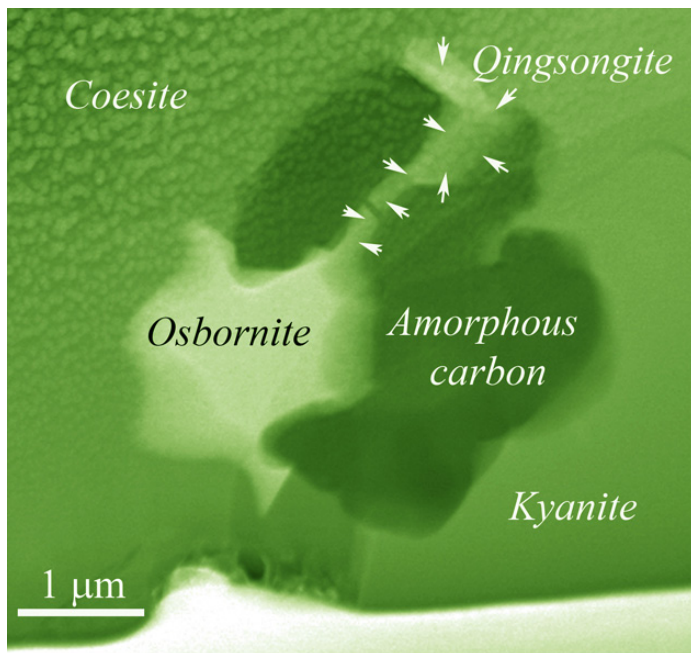
### LLNL TO SUPPORT NEW CENTER FOR BIOLOGICAL XFEL IMAGING



With a \$25 million grant from the National Science Foundation, a consortium led by the University of Buffalo will establish the Biology with X-ray Free Electron Lasers (**BioXFEL**) Research Center with its partner institutions, including Lawrence Livermore. BioXFEL is intended to “**transform the field of structural biology**” and will focus on developing new x-ray bioimaging techniques, including an advanced form of x-ray crystallography—called serial femtosecond crystallography—to analyze molecular targets for drug discovery. (A pioneer in the field of biological imaging with XFELs, Livermore has conducted theoretical studies and the first proof-of-concept experiments at soft x-ray laser light sources and has also been a major contributor to the first biological imaging experiments at the Linac Coherence Light Source.) LLNL will contribute to the BioXFEL Center by providing technologies for introducing biological samples and methods for time-resolved measurements for two- and three-dimensional protein nanocrystallography, as well as models to investigate the effect of x-ray damage during such measurements—work supported by a current Laboratory Directed Research and Development (**LDRD**) project led by physicist Matthias Frank. Past LDRD projects have also supported pioneering work in biological imaging with XFELs. The photo shows a sample holder containing protein crystal samples for experimentation at the Linac Coherent Light Source.

### NEWLY DISCOVERED MINERAL, QINGSONGITE, OFFICIALLY RECOGNIZED

The International Mineralogical Association **officially recognized a new mineral** discovered in 2009 by researchers at LLNL (Jennifer Matzel, Peter Weber, and Ian Hutcheon), UC Riverside, the University of Maine, and institutions in China and Germany. The new mineral is named **qingsongite**, after Qingsong Fang (1939–2010), a professor at the Chinese Academy of Geological Sciences. The mineral was found in the southern Tibetan mountains of China in paleoceanic rocks that had been subducted to a depth of 190 miles and recrystallized there. “The uniqueness of qingsongite is that it is the first boron mineral that was found to be formed at extreme conditions in deep Earth,” said UC Riverside geologists Larissa Dobrzhinetskaya. “All other known boron minerals are found at Earth’s surface.” The image shows an inclusion of qingsongite in a coesite–kyanite matrix.





### ADVANCED SIMULATIONS HELP DEVELOP NEW LIGHTWEIGHT ARMOR

A team of LLNL scientists and engineers, in collaboration with **Schott DiamondView Armor** and Oak Ridge National Laboratory, has just completed a DARPA project to develop, model, and test new vehicle armor that is significantly lighter than conventional armor. The new armor, which makes use of novel materials, was optimized with high-fidelity physics-based modeling and simulation. For instance, mesoscale simulations were used to develop enhanced continuum models to better predict how the new materials would respond during failure. The team also developed a hyperelastic fiber composite model to capture the finite strain response of the main energy-absorbing components. The LLNL team consisted of Lee Aarons, Tarabay Antoun, Matt Barham, Doug Faux, Eric Herbold, Mike King, George Mseis (now at LightSail Energy), and Oleg Vorobiev.

### CENTER OF EXCELLENCE AWARD FOR NIF TEAM

On November 19, **James Truchard**, cofounder and CEO of National Instruments (NI), presented Livermore's Mike Flegel and the rest of the Lab Systems Team at the National Ignition Facility with a certificate designating the team as a **LabVIEW Center of Excellence**. This designation has been awarded to only a few organizations in the United States, recognizing those that follow best practices in their use of the **LabVIEW** engineering tools and holding up those Centers of Excellence as a model for other organizations. The photo shows, from left, Livermore's Larry Lagin; NI's Christoph Wimmer, Stefano Concezzi, and Adam Wooderson; LLNL's Haiyan Zhang; Dr. Truchard; Mike; and Livermore's Glenn Larkin, Jordan Meyer, Edward Koh, and Raja Gopal (absent: LLNL's Robert McDonald).



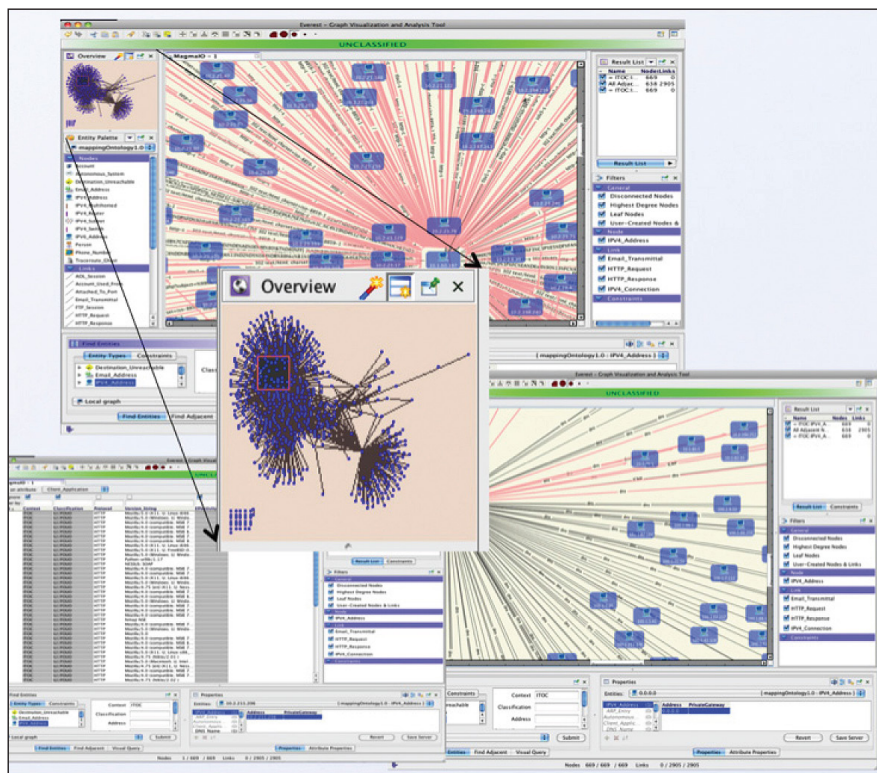


## LABORATORY CONTRIBUTES TO AIR FORCE EFFORT TO IMPROVE COMPONENT DESIGN

Lawrence Livermore is one of the institutions working with the U.S. Air Force (USAF) to ensure that the USAF stays on the cutting edge of global security **improving the safety and fuel-efficiency of aircraft**. Joining other national laboratories, universities, and companies, LLNL is working with engineers at the **Air Force Research Laboratory** to advance the design of aircraft systems by modeling defects and studying materials at the grain level. Leveraging its strengths in computational materials and high-performance computing, the Laboratory is contributing “to tools that convert the raw experimental measurements into physical aspects of material response and their evolution under loading, which facilitates tuning future experiments as well as the overall insights gained.” Livermore’s work was supported in its early stages by the **LDRD** Program.

## CHEMICAL SECURITY PERSONNEL SUPPORT STATE DEPARTMENT TRAINING FOR TURKEY

As lead laboratory supporting the U.S. State Department for chemical security and forensics training in the Middle East, Livermore sent Armando Alcaraz and Eileen Vergino to two laboratories in Turkey. The LLNL researchers evaluated the physical capacity of the laboratories—in Ankara and Bursa—in preparation for a course to be designed to help Turkey in proficiency testing related to the **Chemical Weapons Convention**. Actual course design will be conducted at the Finnish Institute for Verification of the Chemical Weapons Convention. In addition to this course, Turkish participants will also attend training at LLNL, which will focus on the Laboratory’s strong capabilities in chemical weapons analysis, such as its status as one of only two U.S. laboratories certified under the Organization for the Prohibition of Chemical Weapons.



## CYBER TOOL PITCHED TO VENTURE CAPITALISTS BY HOMELAND SECURITY

An LLNL cybersecurity tool was one of eight cutting-edge technologies **showcased to Silicon Valley venture capitalists** under the Department of Homeland Security’s **Transition to Practice Program**. The tool, Net\_Mapper (left), is designed to find anything attached to a network—devices, open ports, communication paths, routing directives, and the processing of transactions between hosts and users of the network. Said Michael Pozmantier, manager of the Transition to Practice Program, “They like to say [Net\_Mapper] finds everything you expect and more.” Net\_Mapper received crucial early-stage support from the LDRD Program through the Continuous Network Cartography Project (13-SI-004).

### MICROBIAL DETECTION TECHNOLOGY AIDS SKELETON-SLEUTHING ANTHROPOLOGISTS

When a team of anthropologists investigating a church graveyard in Altopascio, Italy, needed help determining the cause of death of unidentified skeletons, they turned to Lawrence Livermore. As **reported in *Science***, the anthropologists asked to have genetic samples analyzed with the Lawrence Livermore Microbial Detection Array (**LLMDA**), which is now being used to scan the samples for genetic indicators of any of the approximately 6,000 species that the current version of the technology can detect—3,111 viruses, 1,967 bacteria, 94 protozoa, 136 fungi, and 126 archaea (primitive bacteria). If LLMDA detects the cholera bacterium—*Vibrio cholerae*, currently the prime suspect for one group of burials—then this will enable the investigators to compare the genome of that particular strain to those of strains known today. LLMDA was also recently **used in a milestone bladder cancer study** and has also been the subject of a cooperative research and development agreement **with a Danish public health organization**. In the realm of commercialization, LLMDA's recognition includes an **Outstanding Technology Award** from

the Federal Laboratory Consortium, and the technology **has been licensed** to a Missouri-based supplier DNA microarrays and instruments. The photo shows a skeleton being excavated at the Altopascio churchyard, where **burials began** almost 1,000 years ago. DNA samples sent for analysis with Livermore's LLMDA were taken from the skeletons' teeth.

### IPHONE APP FOR LLNL-DERIVED GLUCOSE-MONITORING SYSTEM

Global technology company Sagentia recently announced it had developed a medically regulated iPhone application for the Senseonics Glucose Monitoring System to provide self-management assistance to diabetes patients. The Senseonics Glucose Monitoring System is based on an LLNL technology—“Long-Wavelength Fluorescence Quenching Sensor for Measuring an Analyte such as Glucose”—and consists of three major components: an implanted sensor, a wireless transmitter that communicates with the sensor, and a smartphone mobile medical application. After insertion, the system functions noninvasively, automatically, and continuously for six months or longer, measuring a patient's glucose

levels every few minutes and sending accurate, specific alerts to both the user and his or her physician about impending hyperglycemia or hypoglycaemia. Sagentia brought to the project its expertise with Bluetooth low-energy connectivity, enabling extremely fast and reliable communication between the smartphone application and the embedded device.





### LAB CONTRIBUTES TO SCIENTIFICALLY ACCURATE, SIMULATION-RICH QUAKE EXHIBIT

A major exhibit at the California Academy of Sciences in San Francisco **incorporates Lawrence Livermore simulation results** to create an engaging yet scientifically accurate exhibit. “**Earthquake: Evidence of a Restless Planet**” was produced in collaboration with scientific and science education advisory panels and nearly 100 contributors from research institutions, **including LLNL**, the U.S. Geological Survey, and the University of California at Berkeley. The core of the exhibit is a half-hour film, *Earthquake*, that features striking visualizations of quakes, tsunamis, and tectonic plate evolution. One of the film’s goal is to teach the public that scientists



use not only field observations but also computational models and simulations to understand Earth’s behavior. Consequently, *Earthquake* features 20 visuals generated directly from scientific data—more than any previous Academy of Sciences film—including some drawn from LLNL seismic research, such as accurate ground-motion simulations for two major earthquakes (one historical and the other hypothetical), simulations of seismic waves traveling through Earth, and a temperature map of Earth’s interior based on global seismic-wave imaging. Laboratory seismologist Arthur Rodgers (shown at the exhibit in the photo) led the Livermore “Earthquake” exhibit collaboration team, which included Christina Morency, Nathan Simmons, Anders Petersson, and Bjorn Sjogreen.

### LLNL SUPERCOMPUTING RECOGNIZED AT CONFERENCE

At the Supercomputing 2013 (**SC13**) conference, held recently in Denver, Colorado, LLNL was presented with a Reader’s Choice Award from HPCWire in the category of “Best Application of Green Computing in High-Performance Computing (HPC)” in recognition of the Laboratory’s efforts to make its HPC facilities as energy efficient as possible. The Laboratory also received an Editor’s Choice Award in the category “Best HPC Collaboration Between Government and Industry” in recognition of its outreach to industry through the **High-Performance Computing Innovation Center** and special programs such as the HPC4energy Incubator.

### SUCCESSFUL LAUNCH OF CUBESAT TO TEST SPACE-JUNK-TRACKING TECHNOLOGY

The Laboratory’s second “cubesat”—a type of miniaturized satellite—**was successfully launched** on a Minotaur rocket from the NASA Wallops Flight Facility on November 19. This cubesat will demonstrate new technologies to track objects in orbit. The cubesat was **launched** as auxiliary payload, along with over 20 other of the shoebox-sized devices.

### STUDENT WINS CAL STATE EAST BAY “BEST THESIS” AWARD

Daniel Segal, an LLNL summer intern and student employee working on the State of California-funded Groundwater Ambient Monitoring and Assessment (**GAMA**) Program, has been named winner of the 2013 Harrington Award for the best M.S. thesis in the College of Science at California State University East Bay. The research for Daniel’s thesis, titled *Dissolved Gases and Isotopes as Tools for Aquifer Characterization in Martis Valley*, was conducted at LLNL, and his thesis advisor at Cal State East Bay was former LLNL employee Professor Jean Moran.

### GRADUATE STUDENT ELECTED AS STUDENT REPRESENTATIVE FOR APS FAR WEST SECTION

Jackson Williams, a UC Davis graduate student who is doing his thesis research at LLNL, was elected to the position of student representative of the **Far West Section** of American Physical Society. At LLNL, Jackson works with staff scientist Hui Chen and others to conduct fundamental research on aspects of intense laser–plasma interactions related to positron–electron pair creation.

### ATMOSPHERIC SCIENTIST APPOINTED TO EERE ADVISORY COMMITTEE

Atmospheric scientist Sonia Wharton has been appointed to the Wind and Water Program Advisory Committee in DOE’s Office of Energy Efficiency and Renewable Energy (EERE). The Committee will help develop a new 7-year DOE initiative dubbed “Atmosphere to Electrons,” which aims to develop methods to optimize the systems-level performance of wind-power plants. The initiative’s scope includes multiscale atmospheric physics, analysis, modeling and forecasting, and wind turbine physics and modeling. Sonia will be a member of the advisory panel for experimental measurement.

### CLIMATE COLLABORATION SELECTED FOR “ENLIGHTEN YOUR RESEARCH” PROGRAM

A research collaboration led by LLNL was one of four selected to participate in the first-ever **Enlighten Your Research Global** program, which seeks to identify global, data-intensive projects that could significantly benefit from enhanced global network connectivity. The proposal “International networking for climate,” led by Livermore’s Dean Williams, will offer researchers the ability to access climate data at replication sites around the world, such as LLNL’s Program for Climate Model Diagnosis and Intercom-

parison (**PCMDI**) and the United Kingdom’s Center for Environmental Data Archival (**CEDA**). The project, whose goal is to boost end-to-end Internet connections between sites to 4 gigabits per second by 2014, is meant to compliment the Earth System Grid Federation (**ESGF**), which Dean also runs. Enlighten Your Research Global was launched by five of the world’s leading national research and education networks, whose executives selected the projects to participate. The selections were officially announced at this year’s Supercomputing Conference (**SC13**), held recently in Denver, Colorado.

### LLNL LICENSEE GOES GLOBAL WITH FORWARD OSMOSIS MEMBRANES

Livermore licensee **Porifera, Inc.**—a Silicon Valley startup that develops advanced membranes for water treatment—announced that it recently entered a development, manufacturing, and commercialization agreement with South Korea’s Woongjin Chemical Company. The investment provided under the agreement will enable Porifera to market, manufacture, and sell its forward osmosis products at high volume while also gaining access to Woongjin’s global sales and marketing channels. Porifera has pioneered development of carbon nanotube membrane technology, licensed from LLNL in 2009, and forward osmosis membranes for water treatment. Porifera anticipates that these membranes will open up large markets, particularly in Asia, for the cost-effective treatment of highly fouling industrial waste waters. A significant North American market opportunity also exists for the treatment of high-fouling waters resulting from hydraulic fracturing. “The Woongjin investment is a huge vote of confidence for bringing this disruptive technology into the commercial mainstream,” said **Olgica Bakajin**, Porifera CEO and former LLNL principal investigator responsible for the research and development of the technology with support from the Laboratory Directed Research and Development (**LDRD**) Program.



### CRADA TO IMPROVE MAPPING OF UNDERGROUND INFRASTRUCTURE

In October, the Laboratory signed a cooperative research and development agreement with **Underground Imaging Technologies, LLC**, to develop improved technology for mapping and imaging underground infrastructure. The Orlando, FL-based small business develops and integrates hardware and software systems for such mapping and provides comprehensive services to construction companies to improve the safety, accuracy, and efficiency of operations related to underground infrastructure, including design, construction, and management.

### LIVERMORE PCR LICENSEE ANNOUNCES EXPANSION

In September, LLNL licensee **RainDance Technologies** announced it had raised \$35 million in financing for commercial expansion. The Billerica, Mass.-based manufacturer of life sciences instruments, which is on track to exceed \$20 million in revenue this year and could hold an initial public offering in 2014, licensed a Livermore technology for nucleic acid detection and analysis in 2008. Two RainDance products incorporating this technology are **Raindrop Digital PCR System** and **ThunderStorm System**, which are used by academic researchers, pharmaceutical companies, and clinicians to detect the presence of disease—primarily cancer, infectious disease, and inherited diseases. The products function as tools with which customers can develop their own tests for a disease.

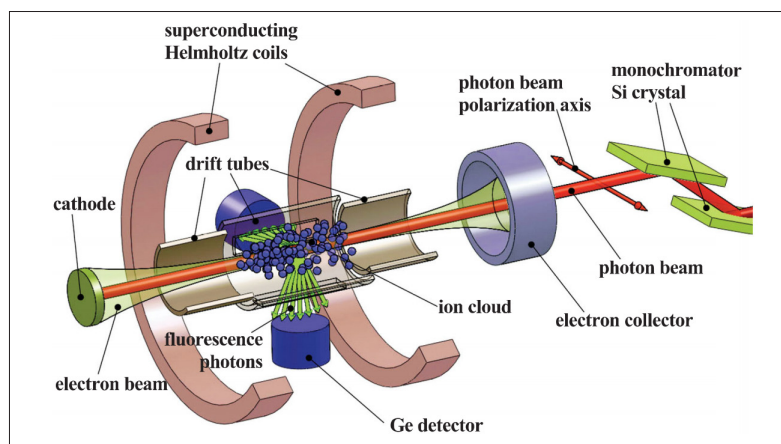
### LIVERMORE AWARDED 1 BILLION SUPERCOMPUTER HOURS UNDER DOE'S INCITE PROGRAM

Under DOE's Innovative and Novel Computational Impact on Theory and Experiment (**INCITE**) Program, seven proposals submitted by LLNL researchers have been awarded more than 1 billion core

hours on two of America's fastest supercomputers dedicated to nonclassified science—**Mira** and **Titan** (respectively located at Argonne and Oak Ridge National Laboratories). The INCITE Program aims to accelerate scientific discoveries and technological innovations by awarding resources on a competitive basis; this year, nearly 6 billion core hours were awarded to a total of 59 projects. The Laboratory's seven projects include David Bader and Stephen Klein's "High-Resolution Simulation for Climate Means, Variability, and Extreme" and Nicolas Schunck's "Nuclear Structure and Nuclear Reactions."

## RESEARCH ON HIGHLY CHARGED IRON SPECTRUM IS *PRL* “EDITORS’ SUGGESTION”

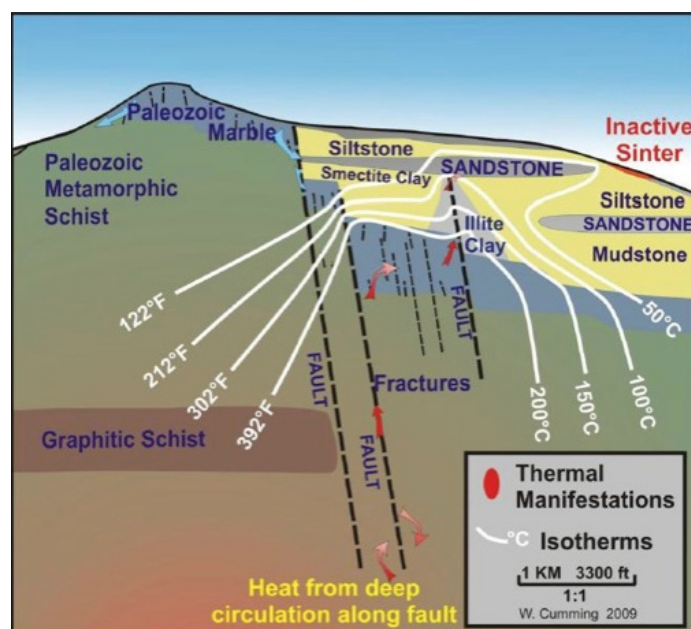
Absorption and fluorescence due to K-alpha transitions in highly charged iron ions are essential mechanisms for the transfer of x-ray radiation in astrophysical environments. In an “Editors’ Suggestion” paper in *Physical Review Letters*, LLNL physicist Greg



Brown, former LLNL postdoc Alex Graf, and colleagues from the University of Maryland and several German institutions **report on photoabsorption due to the main K-alpha transitions** in highly charged iron ions, from heliumlike  $\text{Fe}^{24+}$  to fluorinelike  $\text{Fe}^{17+}$ . The team used a high-fluence monochromatic x-ray beam at Germany’s **PETRA III** synchrotron photon source to excite iron ions in an electron beam ion trap, determining the transition energies and natural linewidths with unprecedented accuracy. These results will be particularly useful for interpreting astrophysical x-ray spectra, especially from active galactic nuclei and high-mass x-ray binary stars, in which absorption and reflection of x-rays from an accretion disk are directly related to the physical properties of the system. These data will also be essential for benchmarking theoretical calculations of atomic structure and spectral models used to interpret spectra from celestial sources. The figure shows the team’s experimental setup, in which germanium photon detectors register fluorescence emission arising from the resonant excitation of  $\text{Fe}^{24+}$  ions by a monochromatic x-ray beam.

## BEST PAPER AWARD WON AT GEOTHERMAL RESOURCES COUNCIL ANNUAL MEETING

Geophysicist Whitney Trainor-Guitton and colleagues at LLNL, the National Power Company of Iceland, and Chevron-Texaco received a Best Paper Award at the Geothermal Resources Council Annual Meeting—held in Las Vegas, NV, from September 29 to October 10—for their paper titled “Value of spatial information for determining geothermal well placement.” The peer-reviewed conference paper presents a methodology for determining the value of various types of geophysical data in the exploration of hidden geothermal resources. Specifically, the methodology can help answer questions such as, Where should we drill to get the most valuable information? The figure below is a conceptualization of a “blind” geothermal resource—i.e., a situation in which no surface feature exists to demonstrate existence of a possible resource.





## A “FIRST” ON LASER-DRIVEN X-RAY SOURCE FOR MATERIAL CHARACTERIZATION RESEARCH

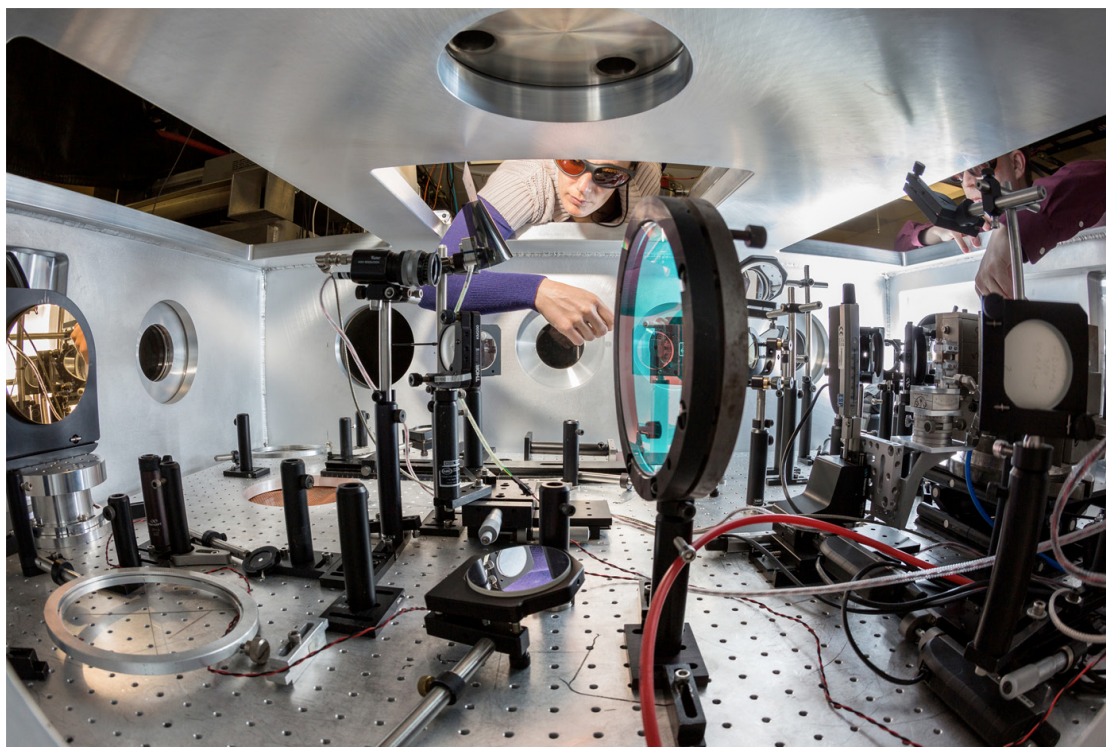
In a paper published in *Physical Review Letters*, Livermore scientist Felicie Albert and colleagues at LLNL, UCLA, and the Stanford Linear Accelerator Center present the first-ever measurements of the angular dependence of the betatron x-ray spectrum generated using a laser-wakefield accelerator (LWFA). The team performed experiments at LLNL’s Jupiter Laser Facility, using the 200-Terawatt Callisto laser system, and then used simultaneous spectral and spatial analysis of the resulting x-rays to reconstruct the electron trajectories within the laser wake field with micrometer resolution, finding an angular dependence that strongly indicates anisotropy (i.e., direction dependence) in these electron trajectories. This finding has significant implications in fusion energy research and other areas of high-energy-density research that use a LWFA to generate matter-probing x-rays as a laser-driven alternative to very large and very expensive free-electron particle accelerators. This work by Felicie et al. was supported by the LDRD Program. The photo shows Felicie (center)

and LLNL colleague Bradley Pollock (far right) preparing the Callisto laser system for betatron x-ray experiments at LLNL’s Jupiter Laser Facility.

## REVIEW OF LASER-PLASMA INTERACTION IN INDIRECT-DRIVE FUSION

An analysis of laser–plasma interaction data from the first complete series of coupling experiments in ignition-scale hohlraums on the National Ignition Facility (NIF) indicates that plasma instabilities could be controlled to maximize coupling and shows they can be beneficial in controlling drive symmetry by precisely adjusting wavelengths of the different beams. In a paper in *Plasma Physics and Controlled Fusion*, lead author Robert Kirkwood and colleagues at LLNL and LANL write that **an understanding of the initial hohlraum coupling experiments is critical**, as they are the first step in a campaign to study indirectly driven implosions under the conditions of ignition by inertial confinement at NIF, and in the near future are likely to further influence ignition plans and experimental designs. The researchers said

the advent of experiments with ignition-scale hohlraums and laser energies up to 1.3 megajoules at NIF “has provided a substantial advance in our understanding of the effects of plasmas on hohlraum coupling and has given us a demonstration that hohlraums can produce x-ray drive with the intensity and uniformity that is needed to implode capsules at the scale expected to be necessary to ignite fusion reactions.”



## IN SIMULATION-EXPERIMENT MILESTONE, HOW EXPLOSIVES RESPOND TO SHOCKWAVES

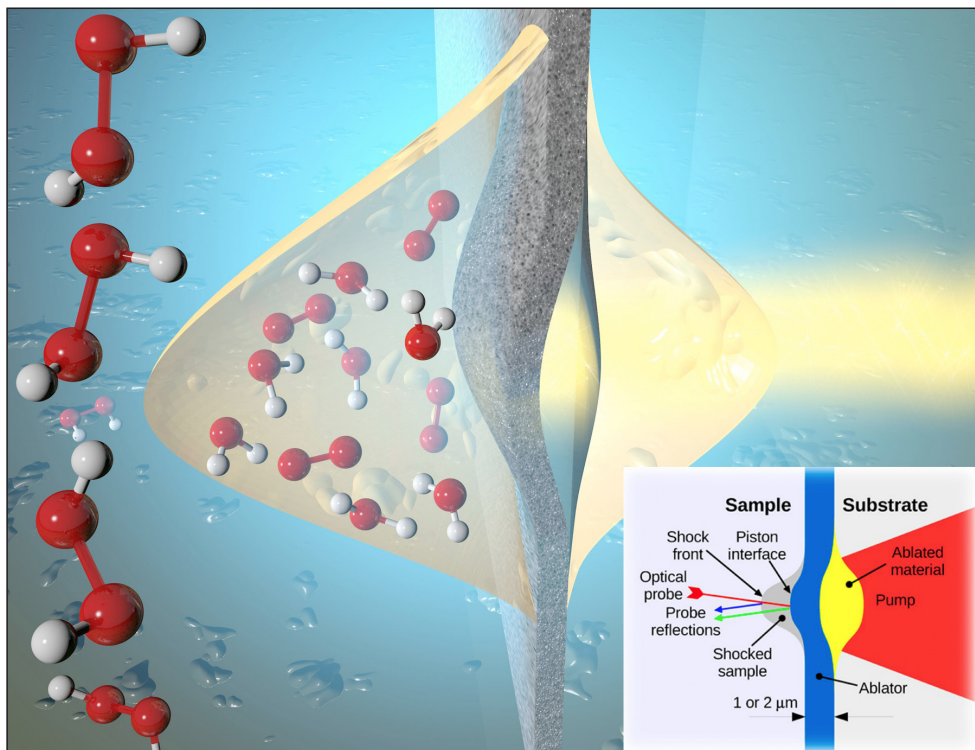
In a milestone in understanding chemical initiation and detonation, LLNL researchers investigating the explosion of an energetic material—hydrogen peroxide—using molecular dynamics (MD) simulations and ultrafast experimental shock wave methods achieved agreement between both at an ultrafast timescale. The results—**published in the *Journal of Physical Chemistry A***—include experimental data indicating initiation of the hydrogen peroxide within 100 picoseconds of arrival of a shock wave, which was consistent with the MD simulations. “What is unique about this research effort is that we have ultrafast, time-resolved experimental data that corroborate our theoretical predictions on the exact same timescale,” said **Nir Goldman**, who helped lead the simulation effort. Project leader **Sorin Bastea** remarked, “This is a step forward where eventually we can have a better understanding of how to control the delivery of chemical energy for a variety of energetic materials applications.” This work **was supported** by Livermore’s Laboratory Directed Research and

Development (**LDRD**) Program. The figure shows a representation of the simulation and experimentation (see **video**), in which detonation was triggered with a laser pulse fired into a thin aluminum film in contact with the hydrogen peroxide.

## LLNL SCIENTISTS FIND LINK BETWEEN GLOBAL WARMING AND RAINFALL CHANGES

A study by Livermore scientists published in *Proceedings of the National Academy of Sciences* shows that **observed changes in global precipitation are caused by human activities**. The authors explain that emissions of heat-trapping and ozone-depleting gases affect the distribution of precipitation through two mechanisms: thermodynamic changes, in which increasing temperatures make wet regions wetter and dry regions drier, and changes in atmospheric circulation patterns that push storm tracks and subtropical dry zones toward the poles. The team compared climate model predications with observations from the **Global Precipitation Climatology Project** and found that natural variability (such as El Niños) did

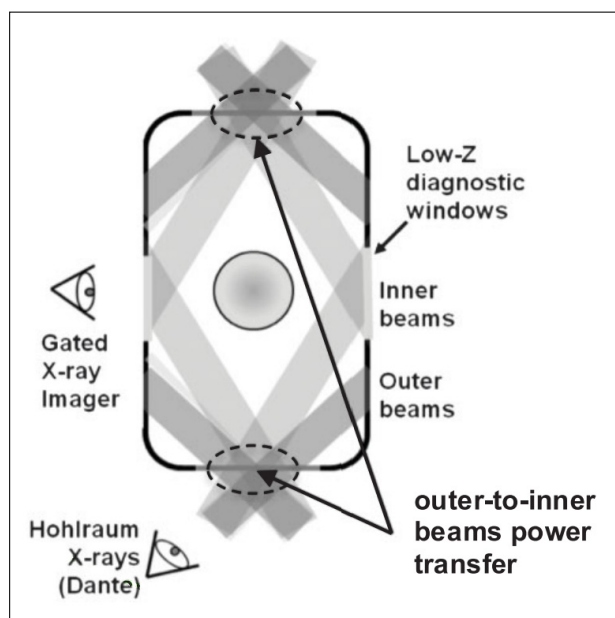
not account for the changes in global precipitation patterns. “In combination, manmade increases in greenhouse gases and stratospheric ozone depletion are expected to lead to both an intensification and redistribution of global precipitation,” said LLNL co-author **Céline Bonfils**. Said lead author Kate Marvel: “Most previous work has focused on either thermodynamic or dynamic changes in isolation. By looking at both, we were able to identify a pattern of precipitation change that fits with what is expected from human-caused climate change.”





## NIF EXPERIMENTS REPORTED IN PRL PAPERS

Recent experimental campaigns on NIF aimed at increasing the compression and improving the symmetry of imploding target capsules were reported in papers in *Physical Review Letters*.



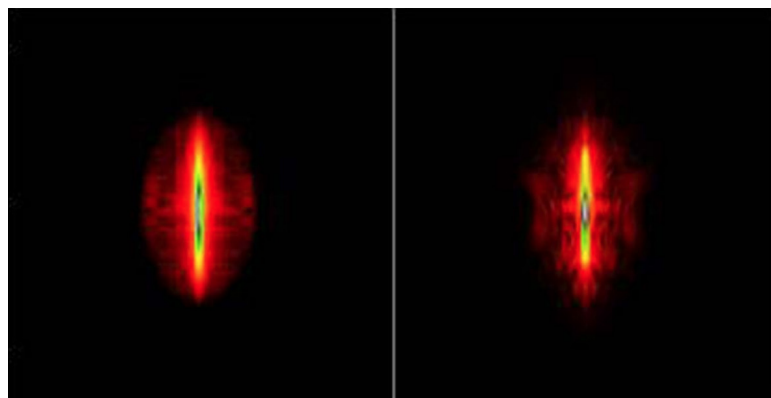
A paper by lead author Vladimir Smalyuk and colleagues at LLNL, the University of Rochester, Massachusetts Institute of Technology, and General Atomics **describes the results** of low-adiabat, cryogenic deuterium–tritium layered plastic capsule implosions. These experiments were conducted to study how sensitive overall performance was to peak laser power and drive duration. New, lower-power, extended-duration laser drives were employed to reduce the duration of the coasting phase of the laser drive, thereby improving fuel compression.

A paper by Eduard Dewald and colleagues from LLNL, LANL, and General Atomics **described the effect of cross-beam energy transfer** (CBET) on early-time hohlraum-driven implosion symmetry. The researchers demonstrated that early-drive asymmetry can be minimized by varying the relative input powers between different cones of beams. The experiments also provided the first time-resolved measurements of CBET in hohlraums, which were in good agreement with radiation-hydrodynamics cal-

culations, including those with a linear CBET model. The figure shows the NIF reemit experimental setup discussed by Eduard and team.

## ULTRAFAST SHORT-PULSE FIBER LASER DESCRIBED

Very-short-pulse laser sources (in the range of picoseconds to femtoseconds) with ultrahigh repetition rates (100 megahertz to tens of gigahertz) have applications as drivers of short-wavelength, high-energy photon sources and in high-frequency particle accelerators. Other applications include three-dimensional lithography, high-data-rate laser communication, and remote sensing systems. In a paper in *Optics Letters*, LLNL researchers **report their development of a unique 11-GHz fiber laser system** built on a modulated continuous-wave platform. The compact, vibration-insensitive system can be operated at wavelengths compatible with high-energy fiber technology. The system is directly driven by a radio-frequency signal and is tunable over a wide range of drive frequencies. Say the authors: “We believe this technique may lead to a new class of oscillators with extremely high repetition rates . . . that provide an extremely stable and robust alternative to conventional mode-locked oscillators.” Livermore’s Matthew Prantil and other were joined by colleagues at France’s University of Bordeaux. The **LDRD** Program supported this work at Livermore. The figure shows measured (left) and retrieved (right) traces of the 11.4-GHz pulse train in a frequency-resolved optical gating.



## NEW DEVICE CREATES HYDROGEN FUEL FROM SUNLIGHT AND WASTEWATER

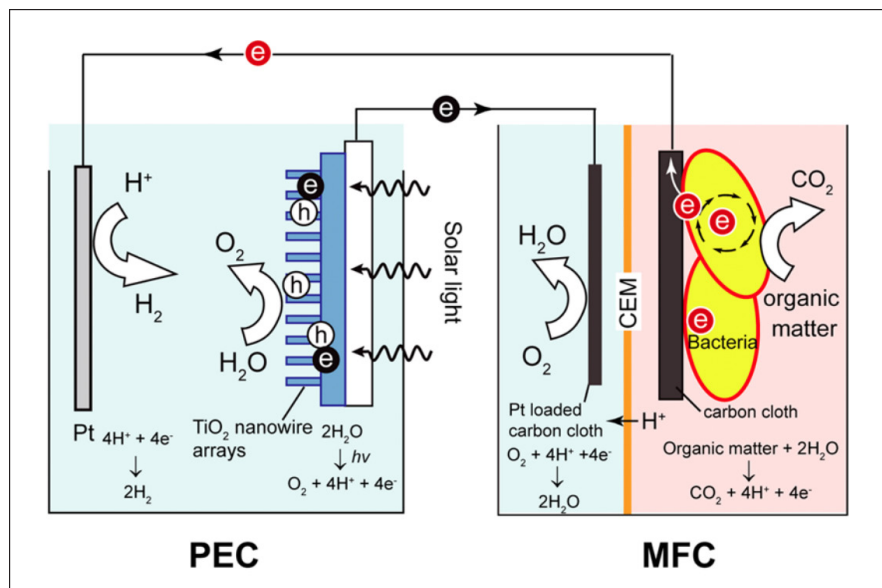
Livermore postdoc Fang Qian and staff biologist Yongqin Jiao, along with colleagues from UC Santa Cruz and the Virginia Polytechnic Institute, have created a new device **that produces hydrogen gas using only sunlight and wastewater**. Described in a paper in *ACS Nano*, the device, if proven scalable, could provide a sustainable energy source while improving the efficiency of wastewater treatment. The new device combines a microbial fuel cell (MFC) and a type of solar cell called a photoelectrochemical cell (PEC). In the MFC portion of the system, electrogenic bacteria—which transfer metabolically generated electrons across their cell membranes to an external electrode—degrade organic matter in the wastewater, generating electricity in the process. The biologically generated electricity is delivered to the PEC part of the system to assist the solar-powered splitting of water (electrolysis), which generates hydrogen and oxygen. Either a PEC or MFC device can be used alone to produce hydrogen gas, but both require a small additional voltage to overcome the thermodynamic energy barrier associated with reducing protons to hydrogen. Providing this additional electric power element adds significantly to the cost and complication of implementing such energy-

conversion systems, especially at large scales. In comparison, the new hybrid solar–microbial device is self-driven and self-sustained because the combined energy in the organic matter in the wastewater (harvested by the MFC) and sunlight (captured by the PEC) is sufficient to drive electrolysis of water. The figure is a schematic illustration of the new hybrid PEC–MFC device. This work was supported by the **LDRD** Program.

## REACTION MECHANISM COULD REVOLUTIONIZE ENERGY CONVERSION AND STORAGE

In a paper published in *Journal of the American Chemical Society*, LLNL researchers Brandon Wood and others use state-of-art computer simulations to **demonstrate a synergetic effect between an electrode surface and a catalyst** at the electrode's surface whereby long-range proton transfer along the surface increases overall reaction efficiency much more than the catalyst alone. This finding suggests a new paradigm for designing energy conversion and storage devices and implies that the assembly of nanoscale device components into a structured mesoscale architecture will result in conversion efficiencies far better than previously achievable. To advance this approach, Brandon is developing a mesoscale

simulation method that will elucidate the nature of the interplay between nanoscale elements in a mesoscale or macroscale device and potentially serve as a tool for designing future devices. This work was supported by the DOE Energy Fuel Cell Technologies Program.





## METEORITE MINERALS GIVE CLUES TO SUPERNOVA THAT CREATED SOLAR SYSTEM

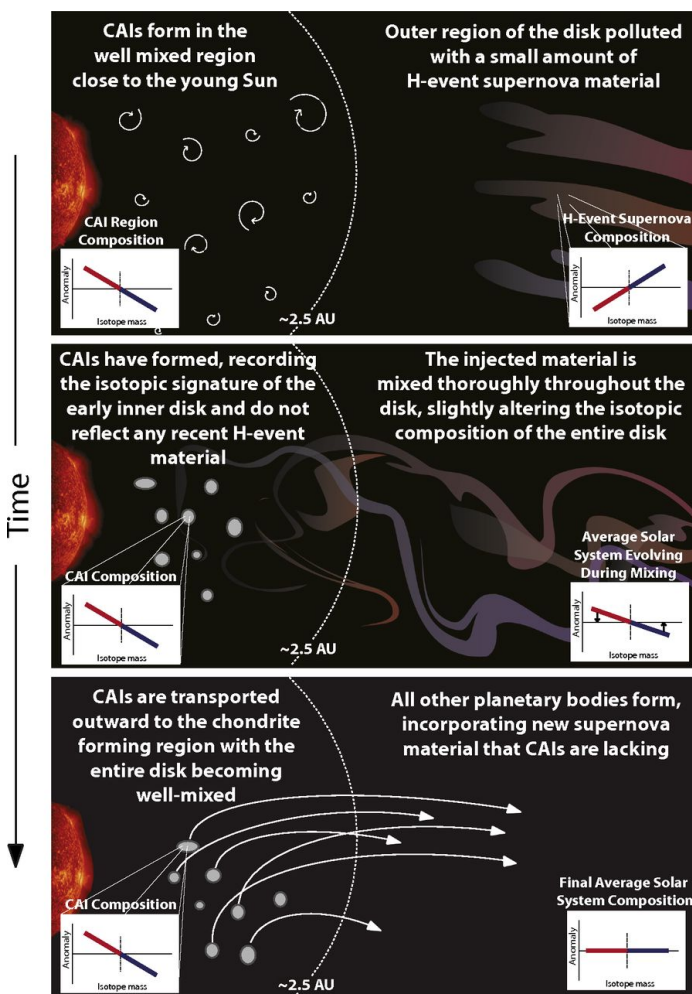
Gregory Brennecka and Lars Borg of LLNL and colleague Meenakshi Wadhwa of Arizona State University examined calcium–aluminum-rich inclusions (CAIs) found in meteorites. CAIs consist of minerals that are among the first solids condensed from a high-temperature gas that existed in the protoplanetary disk at the earliest stages of our solar system’s formation. The team, publishing in *Proceedings of the National Academy of Sciences*, **found that the inclusions had different heavy isotope fingerprints** from younger rocks from Earth, Mars, or the Moon. “That means a supernova must have sprinkled elements with different composition of heavy isotopes into the solar system sometime between the formation of the first solids [CAIs] and the formation of the

planets,” said Gregory. This difference “gives us a time window for when the supernova would have occurred. And it tells us that the neighborhood we were growing up in was rough.” The figure is a schematic explaining how the isotopic signatures of CAIs were “locked in” before the mixing of later material in the solar system, thereby differing from what today is the average solar system isotopic composition.

## EFFICIENCY OF LASER-TO-X-RAY CONVERSION INCREASED

Bright x-ray sources (of several thousand electron-volts) are needed for imaging and radiography applications with large homogeneous sources being useful for area back-lighters, while very bright sources can be used for point-projection back-lighters. In addition to brightness, x-ray sources across a range of energies are needed for studies of x-ray interaction with materials. For this reason, maximizing the laser-to-x-ray conversion efficiency and tuning the spectral content of the x-ray source are crucial to satisfying the requirements of any backlighter or material interaction application.

In *Physical Review E*, Livermore’s Kevin Fournier and colleagues, along with a collaborator at the University of Rochester, report their **demonstration of a significant enhancement of laser-to-x-ray conversion efficiency** from krypton-gas-filled targets. Their results represent a new record for both flux and total energy emitted by a 13-keV source. Experiments on NIF, using about 25 times more laser energy than previous experiments, have created near-optimal conditions for krypton K-shell x-ray emission, they reported. The experiments demonstrated that the x-ray environment generated on NIF with a krypton-gas-filled target irradiated with 0.7 megajoule of laser energy achieves a laser-to-x-ray conversion efficiency into krypton K-shell emission that is an order of magnitude greater than the results of similar experiments on the OMEGA laser.



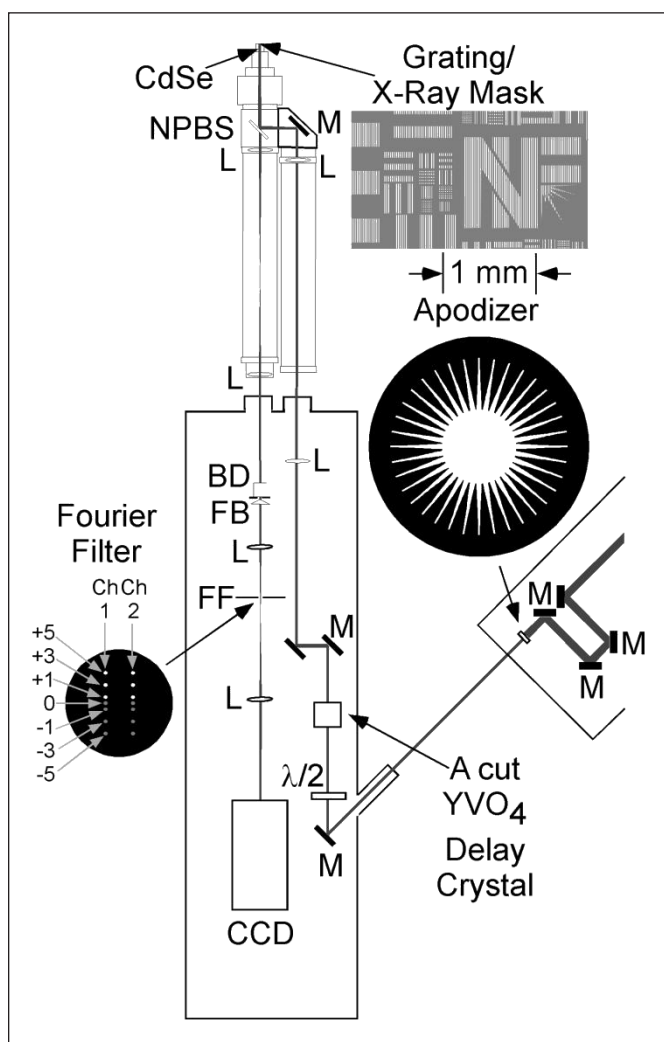
## NEW SOLID-STATE FRAMING CAMERA WITH MULTIPLE TIME FRAMES

A new **high-speed solid-state framing camera** that can operate over a wide range of photon energies is described by Kevin Baker and other LLNL researchers in a paper in *Applied Physics Letters*. The camera, which measures the two-dimensional spatial profile of the flux incident on a cadmium selenide semiconductor at multiple times, has been tested at 3.1 eV and 4.5 keV. Unlike previous cameras based on microchannel plate technology, the device uses only optical and solid-state components to achieve the functions of a framing camera. Advantages to this approach include higher spatial resolution, temporal resolution approaching 100 femtoseconds, potentially

higher dynamic range, and the ability to operate in a high-neutron-flux environment. The framing camera currently records two frames with a temporal separation between the frames of five picoseconds. This separation can be varied between hundreds of femtoseconds up to nanoseconds, and the number of frames can be increased by angularly multiplexing the probe beam onto the cadmium selenide semiconductor. The figure shows the experimental geometry used to measure the two-dimensional x-ray flux produced by the laser-plasma source at two separate times.

## NEW MD CALCULATIONS OF CHARGED-PARTICLE STOPPING

The rate at which charged particles slow down as they interact with matter is an important indicator of the underlying particle interactions, and simulations of this process help test the accuracy of models of important processes of energy and particle flow, such as thermal conductivity and diffusion. In a paper published in *Physical Review Letters*, LLNL researchers Michael Surh, David Richards, and Frank Graziani, along with colleagues from LANL, **report the results of large-scale molecular dynamics (MD) simulations** of charged-particle stopping in a classical electron gas. Calculations simulated approximately  $10^4$  to  $10^6$  particles (orders of magnitude more than in previous studies) and spanned a range of coupling regimes, from weak to moderately strong, allowing the team to evaluate various stopping-power models currently in use and to determine the ranges over which the models' predictions are valid. Guided by their MD results, the team developed a new model form that agrees with the best existing theory in the weakly coupled regime and also extends into the strongly coupled regime. This work—significant because it shows how large-scale MD simulations can be used to extend plasma theory—was supported by an **LDRD** project led by Frank; the stopping-power calculations, particularly in the weakly coupled regime, were conducted on the Sequoia supercomputer during its initial “shakedown” period before its transition to classified work.





## NANOLIPOPROTEIN CONSTRUCTS MAY PROVIDE BROAD-SPECTRUM DEFENSE AGAINST PATHOGENS

In a paper appearing in *Biomaterials*, a team of Livermore scientists and colleagues from the University of Rochester and BD Biosciences report that molecules known to stimulate the immune system **are significantly more effective when incorporated into nanolipoprotein particles (NLPs)**. This increase in the stimulatory and protective properties of immunostimulatory molecules was demonstrated in both mouse and humans model systems. Most significantly, the team demonstrated that pretreating mice with these NLP constructs can confer protection from an otherwise lethal influenza challenge. The results support the idea that therapies targeting the innate immune system have the potential to provide transient, nonspecific protection from a variety of infectious organisms and underscore the potential of NLPs for enhancing the efficacy of such treatments, with profound potential for biodefense applications. This project, led by Livermore's Amy Rasley, received support from the **LDRD** Program.

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### Questions? Comments?

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